

# **Analysis of a Hydrogen Containment Process for Nuclear Thermal Engine Ground testing**

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# Acknowledgment

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# Introduction

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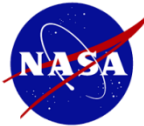
- A safe, robust and affordable hydrogen ( $H_2$ ) removal process is necessary to enable the testing required for nuclear thermal propulsion (NTP) engine development.
- A system-level concept had been developed by burning  $H_2$  and cooling the exhaust with direct water spray. However, it omits first-order physics, creating safety and cost issues concerning the  $H_2$  containment and the large amounts of non-recyclable water.
- A new process is proposed with innovative simplicity that meets design objectives. The process will be demonstrated with high fidelity computational design and analysis tools with innovative physical models.



# Objective

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- The objective of this study is to propose a new total hydrogen containment process to enable the testing required for NTP engine development. This H<sub>2</sub> removal process comprises of two unit operations: an oxygen-rich burner and a shell-and-tube type of heat exchanger. This new process is demonstrated by simulation of the steady-state operation of the engine firing at nominal conditions, with computed hydrogen-to-oxygen ratio at end of heat exchanger less than the lower flammability limit.



# UNIC Multidisciplinary Computational Fluid Dynamics Methodology

- Unstructured-grid, pressure-based, turbulent, finite-rate reacting flow formulation
- Real Fluid Model for multiphase flows

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_j - u_{jg})] = 0 \quad (1)$$

$$\frac{\partial \rho \alpha_i}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_j - u_{jg}) \alpha_i] = \frac{\partial}{\partial x_j} \left[ \left( \rho D + \frac{\mu_t}{\sigma_\alpha} \right) \frac{\partial \alpha_i}{\partial x_j} \right] + \omega_i \quad (2)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_j - u_{jg}) u_i] = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (3)$$

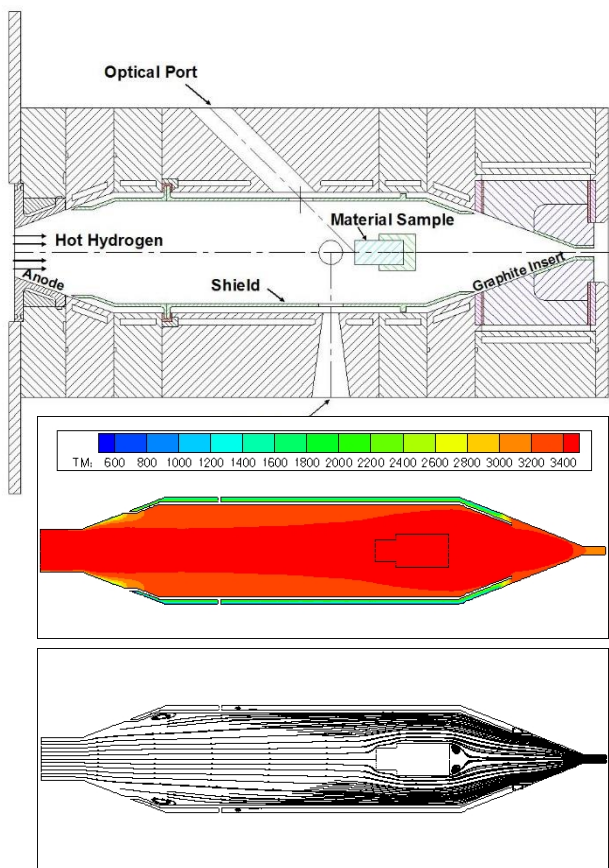
$$\begin{aligned} \frac{\partial \rho H}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_j - u_{jg}) H] = & \frac{\partial p}{\partial t} + Q_r + \frac{\partial}{\partial x_j} \left[ \left( \frac{K}{C_p} + \frac{\mu_t}{\sigma_H} \right) \nabla H \right] + \frac{\partial}{\partial x_j} \left[ \left( (\mu + \mu_t) - \left( \frac{K}{C_p} + \frac{\mu_t}{\sigma_H} \right) \right) \nabla (V^2 / 2) \right] \\ & + \frac{\partial}{\partial x_j} \left[ \left( \frac{K}{C_p} + \frac{\mu_t}{\sigma_H} \right) \left( u_k \frac{\partial u_j}{\partial x_k} - \frac{2}{3} u_j \frac{\partial u_k}{\partial x_k} \right) \right] \end{aligned} \quad (4)$$

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_j - u_{jg}) k] = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + \rho(\Pi - \varepsilon) \quad (5)$$

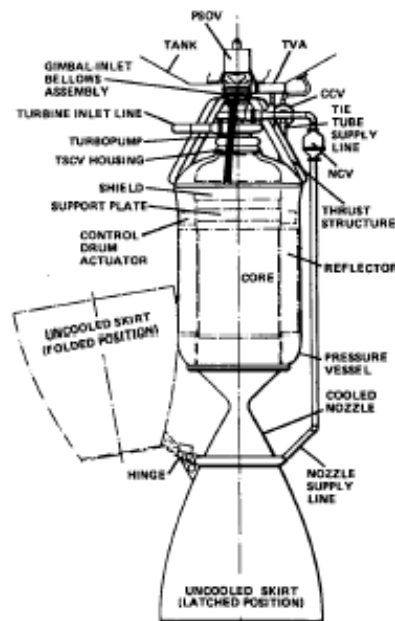
$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_j - u_{jg}) \varepsilon] = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho \frac{\varepsilon}{k} (C_1 \Pi - C_2 \varepsilon + C_3 \Pi^2 / \varepsilon) \quad (6)$$

# UNIC Multidisciplinary Computational Fluid Dynamics Methodology

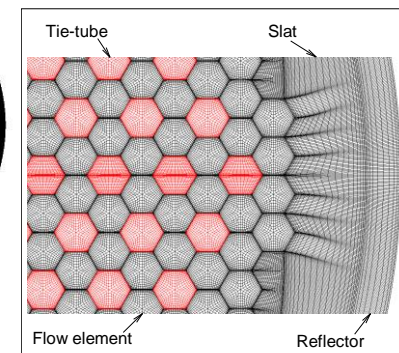
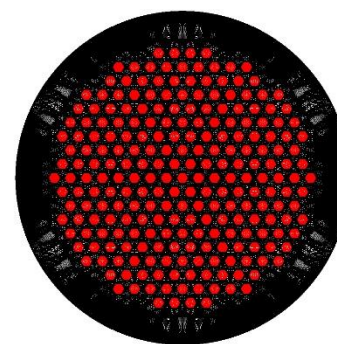
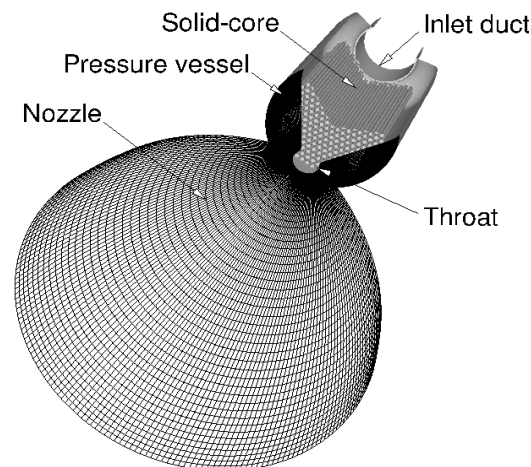
- UNIC has been used to support prior NTP efforts in studying conjugate heat transfer phenomena of a coupon sample being heated in an arc heater, and in a solid-core Small Engine.



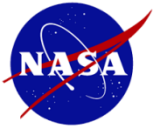
A Cylindrical Specimen Heated by an Impinging Hot Hydrogen Jet



Small Engine



Thrust Chamber Model



# Heat Exchanger Sizing Methodology

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$$\frac{d\rho}{\rho} + \frac{du}{u} = 0$$

$$dp + \frac{4\tau_w dx}{D} + \rho u du = 0$$

$$\dot{Q} = \dot{m} \left( i_2 + \frac{1}{2} u_2^2 - i_1 - \frac{1}{2} u_1^2 \right)$$

The power transfer is calculated with Newton's law of cooling as given by:

$$\dot{Q} = hA(T_w - T_m)$$

The local Nusselt number, used to determine the heat transfer coefficient, is obtained from the Gnielinski equation:

$$Nu_D = \frac{(f/8)(Re_D - 1000)Pr}{1 + 12.7(f/8)^{1/2}(Pr^{2/3} - 1)}$$

Where the Moody friction factor for a smooth wall is given as a function of Reynolds number by the Petukhov equation:

$$f = (0.790 \ln(Re_D) - 1.64)^{-2}$$

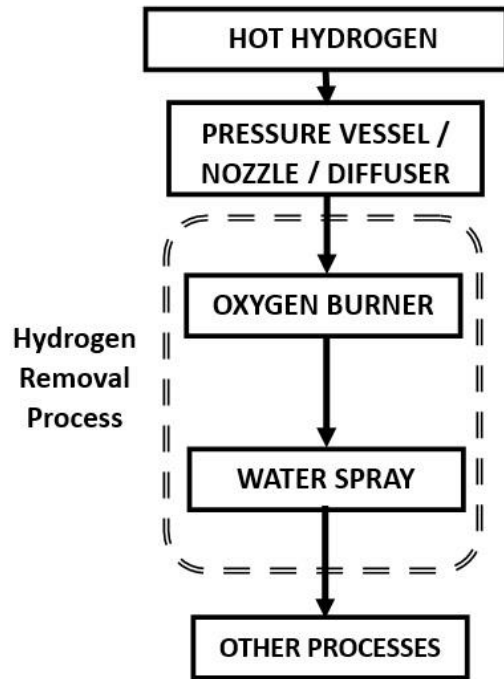
Which is also used to define the wall shear stress as:

$$\tau_w = f \left( \frac{\rho u_m^2}{8} \right)$$

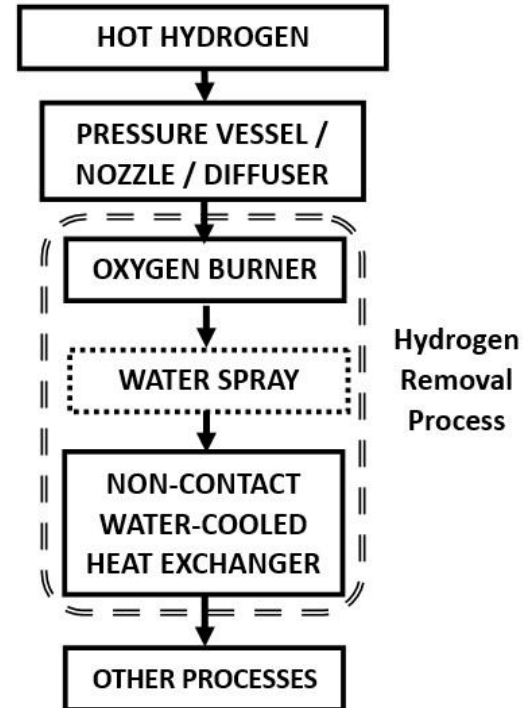
The software Cequel™ (Chemical Equilibrium in Excel), provides the remaining required equation of state functionality and relations for the transport and thermodynamic properties of the combustion gases, which are allowed to dissociate and recombined through the tube assuming equilibrium throughout.



# Total Hydrogen Containment Process

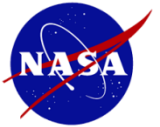


Current process based on system-level model.



The proposed new hydrogen removal process based on the CFD model.





# Conceptual Design

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## Conceptual Design Goals

- Oxygen-Rich Burner design goal: 99% reduction of hydrogen
  - Straight-cylinder burner size
  - State of inlet oxygen
  - O/F ratio
- Heat exchanger design goal: 1% reduction of hydrogen
  - Shell-and-tube tubular heat exchanger
  - Cooling tube size
  - Number of cooling tubes
  - Layout of cooling tubes
- Hydrogen removal process goal: computed flammability < LFL

### Lower Flammability Limit

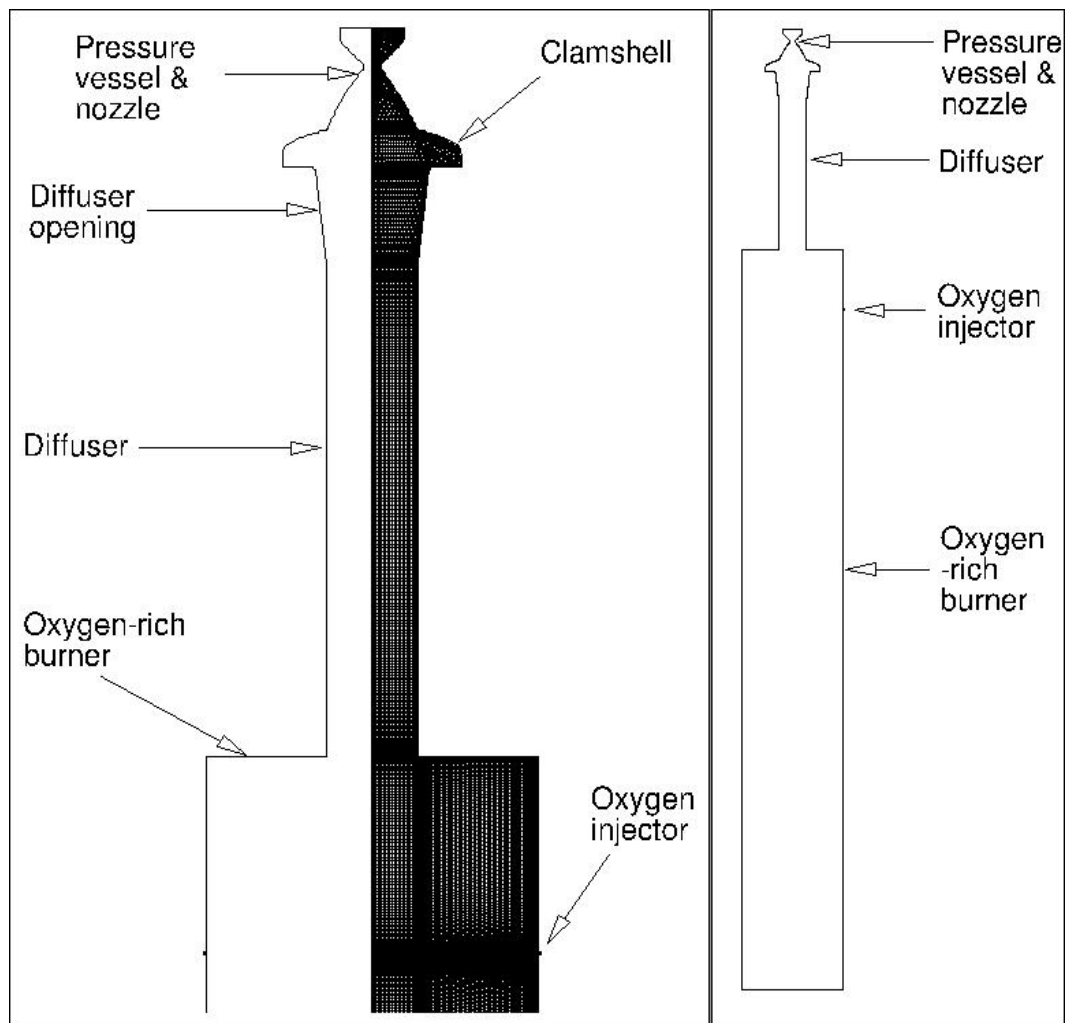
The hydrogen and oxygen mixture can not be ignited if the percent of hydrogen in the mixture (less steam) is less than the lower flammability limit (LFL), or higher than the upper flammability limit (UFL). The flammability limits based on the volume percent of hydrogen in oxygen at 14.7 psia (1 atm, 101 kPa) are 4.0 and 94.0 [25]. Converting to mass percent of hydrogen in oxygen, the LFL and UFL are 0.2618% and 49.67%, respectively. Since the idea of the oxygen-rich burner is to burn off hydrogen as much as possible near the end of the burner, UFL is therefore not applicable and the goal is to reduce the mass of hydrogen in dry mixture to a value lower than the LFL. Note that the auto-ignition temperature of hydrogen is 773 deg. K.

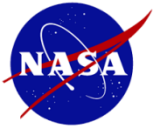
The flammability is calculated as:

$$flammability = \frac{\alpha_{H_2} + \alpha_H + \alpha_{OH}(M_H / M_{OH})}{\alpha_{O_2} + \alpha_O + \alpha_{H_2} + \alpha_H + \alpha_{OH}}$$



# Axisymmetric Grid & Computational Domain





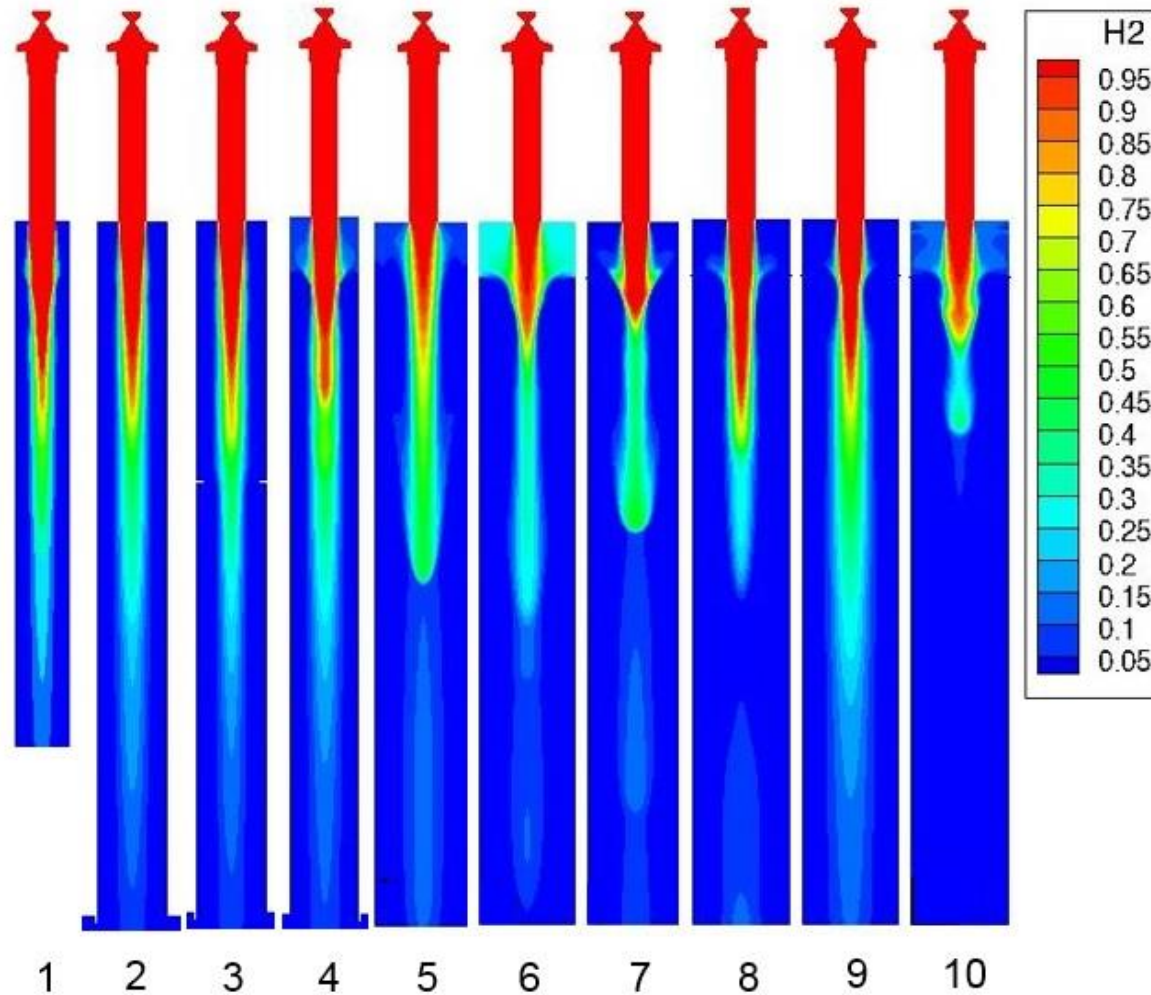
# Axisymmetric, Coupled Pressure Vessel & Nozzle/Diffuser/Burner CFD Parametric Studies

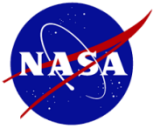
Case	O/F	R/R <sub>o</sub>	L/L <sub>o</sub>	T <sub>O2 inlet</sub> /T <sub>o</sub>	O2 injector geometry	Burner geometry	Ave exit H2 mass fraction, %
1	9	36	705	90	Duct	Straight cylinder	5.81
2	9	46	940	90	Duct	Straight cylinder	3.86
3	9	46	940	90	Duct	Straight cylinder with a long wall fin	3.56
4	9	46	940	300	Sonic nozzle	Straight cylinder	4.27
5	9	65	940	90	Duct	Straight cylinder	3.92
6	9	65	940	200	Duct	Straight cylinder	3.61
7	9	65	940	200	Sonic nozzle	Straight cylinder	4.46
8	9	65	940	300	Sonic nozzle	Straight cylinder	2.58
9	9	65	940	300	Swirled sonic nozzle	Straight cylinder	5.84
10	12.5	65	940	300	Sonic nozzle	Straight cylinder	0.96

This CFD parametric study results show the importance of inter-connected physics such as turbulent mixing, finite-rate chemistry, and residence times that are driven by design parameters such as geometry, O/F ratio, and state of oxygen. It also shows the importance of having a CFD-based process design such that achieving the design objective of the specialized process could be simulated and demonstrated.



# Comparison of H<sub>2</sub> Mass Fraction Contours in Coupled Pressure Vessel & Nozzle/Diffuser/burner CFD Parametric Study



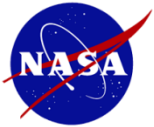


# A Heat Exchanger Sizing Result for a Fixed Cooling Tube Diameter

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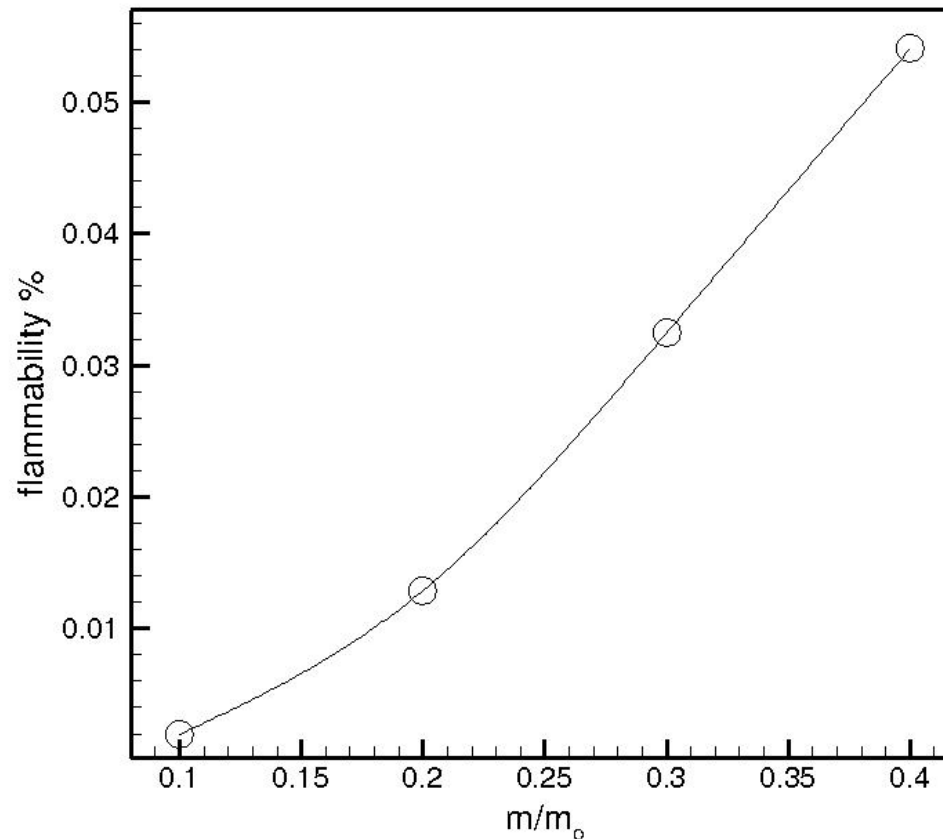
Case	A	B	C	D
$\dot{m}/\dot{m}_o$	1.00	0.50	0.10	0.05
$T_{in}/T_o$	3,331	3,331	3,331	3,331
$T_{out}/T_o$	1,053.5	947.1	733.1	658.0
$T_{wall}/T_o$	400	400	400	400
$D/D_o$	0.1016	0.1016	0.1016	0.1016
$L/L_o$	14.732	14.732	14.732	14.732
$Re_{in}$	114,969	57,485	11,497	5,748
$Re_{out}$	286,453	156,883	39,410	21,771
$Mach_{in}$	0.568	0.284	0.057	0.028
$Mach_{out}$	0.283	0.130	0.023	0.011
$L/D$	145.0	145.0	145.0	145.0

Case C is chosen as a nominal case for the demonstrative computation among many possible cases. The heat exchanger sizing tool is a fast, one-dimensional thermal system model. Although more physics have been added, it still uses assumptions such as equilibrium chemistry. To be conservative and considering those assumptions, the actual  $L/D$  designed was therefore increased from 145 to 230.



# Axisymmetric, Integrated Pressure Vessel & Nozzle/Diffuser/Burner and Single Cooling Tube CFD Results

Case	O/F	$\dot{m}/\dot{m}_0$	Flammability %	Flammability % < LFL?
1	12.5	0.1	0.00193	Yes
2	12.5	0.2	0.01288	Yes
3	12.5	0.3	0.03247	Yes
4	12.5	0.4	0.05406	Yes

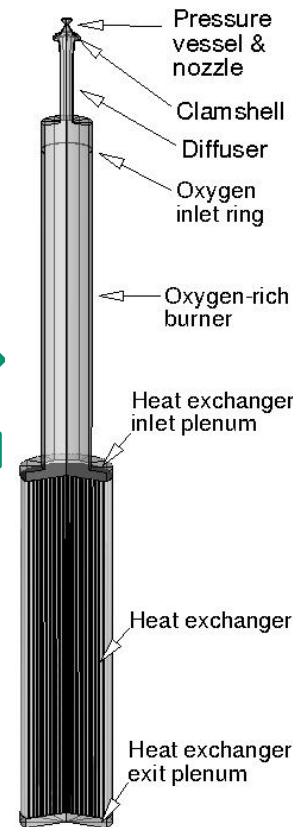
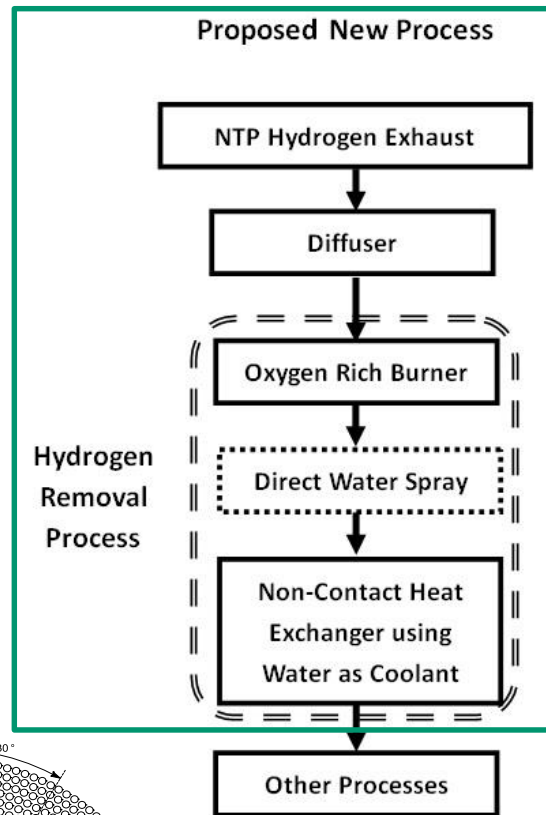


LFL = 0.2618%

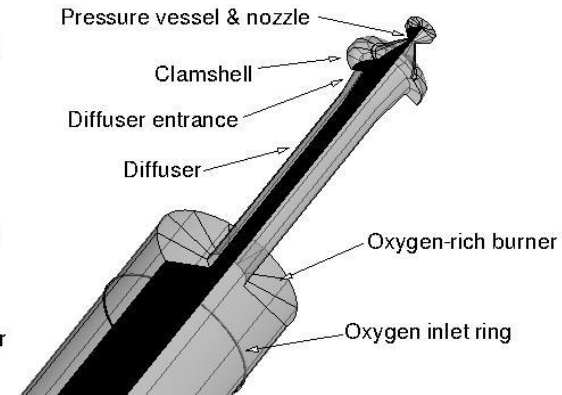




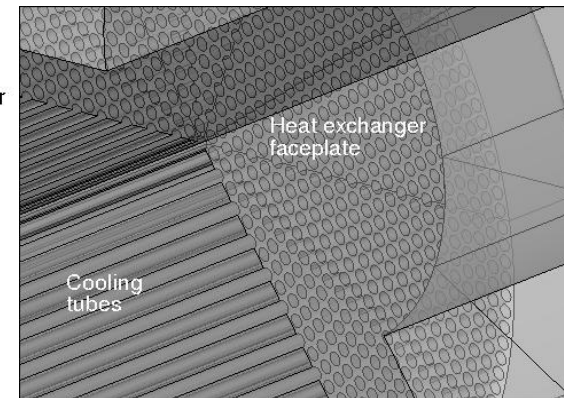
# 3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results



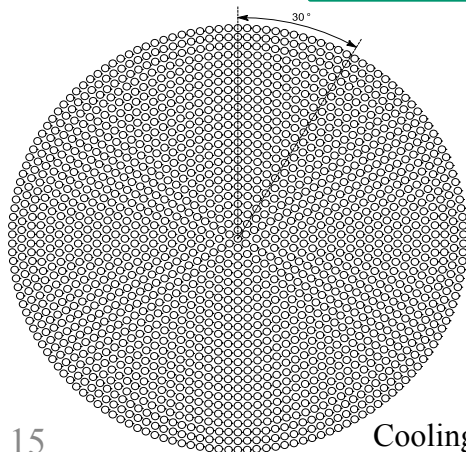
A CFD-based New Process



A close-up view of the layout of NTP engine, nozzle, clamshell, diffuser, and oxygen-rich burner

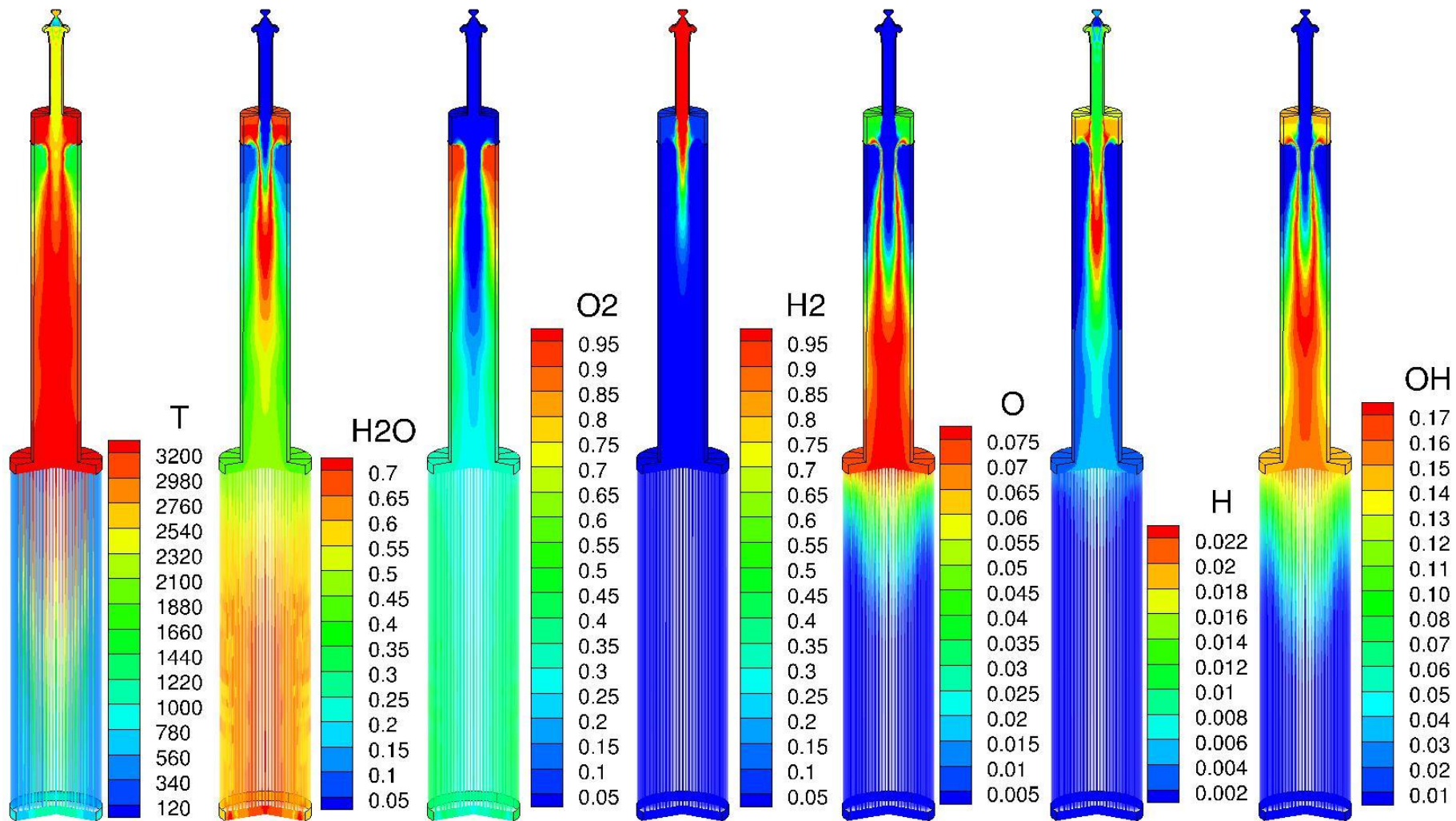


A close-up view of the layout of heat exchanger faceplate and cooling tubes





# 3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results

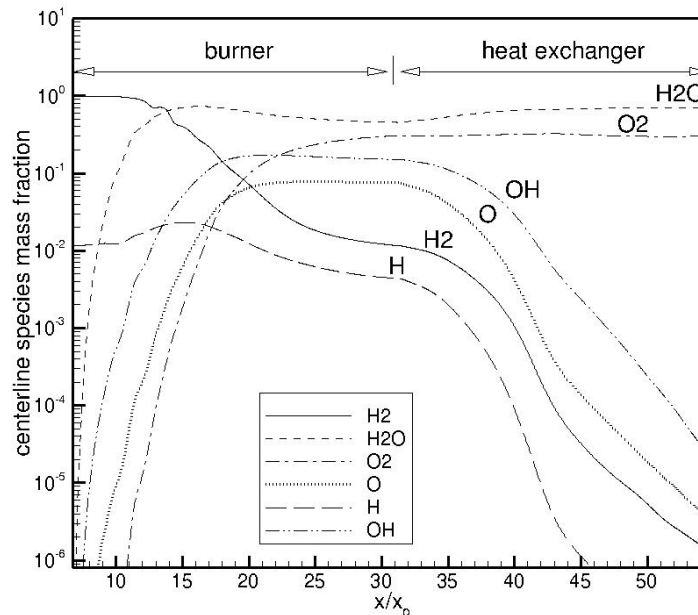
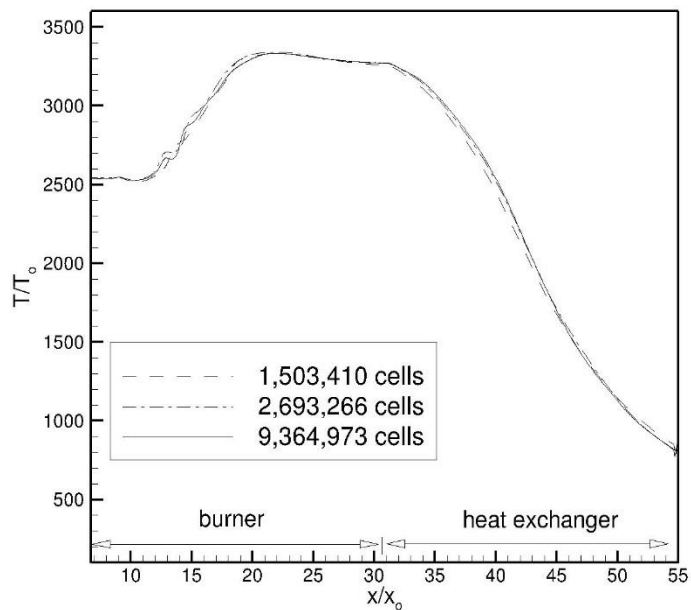


Computed temperature and species concentration contours on the symmetry plane for the entire three-dimensional process

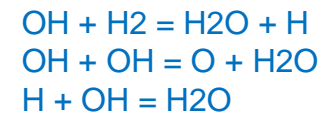




# 3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results



Likely recombination reactions in heat exchanger:



Final flammability computed at the exit plane of the heat exchanger from three grid cell sizes. The flammability results show that H<sub>2</sub> total containment objective has been met with the proposed process.

Case	Cell numbers	Flammability %	Flammability % < 0.2618%?
1	1,503,410	0.00300	Yes
2	2,693,266	0.00204	Yes
3	9,364,973	0.00199	Yes



# Conclusions

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- A new, high fidelity design tools based hydrogen containment process is proposed using a non-contact heat exchanger in lieu of direct water spray for better cooling efficiency and recyclable water (without the need for storing a large amount of water).
- The computed flammability at the end of heat exchanger is less than that of the lower flammability limit, demonstrating the total hydrogen containment capability of the proposed process.